Thioacetamide

62-55-5 | DTXSID9021340

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.38e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.25e-01

Confidence level: 5.27e-01

Nearest Neighbors from the Training Set

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Chloroacetic acid
Measured: 8.49e-02
Predicted: 2.10e-01

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Monuron
Measured: 8.60e-01
Predicted: 2.45e-07

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Ethyl methanesulfonate
Measured: 4.90e-01
Predicted: 4.17e-01

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1,2-Diaminopropane
Measured: 7.00e-03
Predicted: 5.83

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Methyl thioglycolate
Measured: 1.80e-01
Predicted: 2.40